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# Solar wind implantation into lunar regolith: Hydrogen retention in a surface with defects

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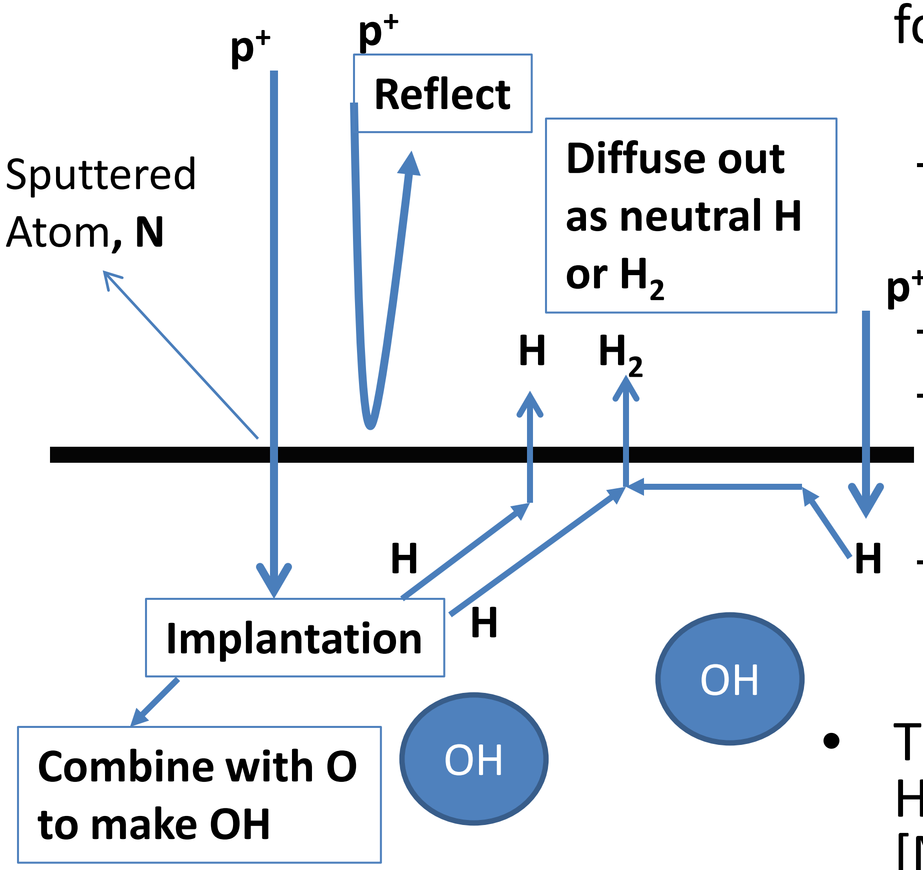
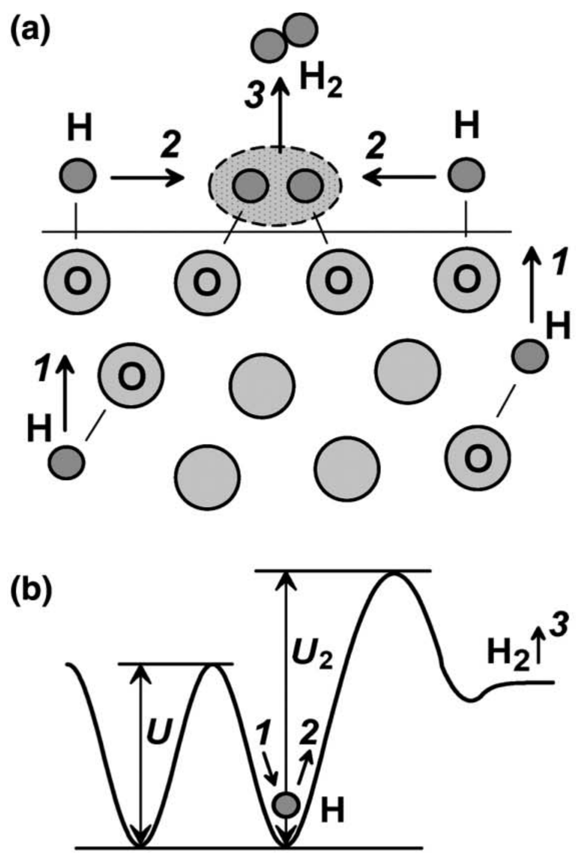
# Proton/surface interaction pathways:




- The end state for proton in surface interactions can be one of the following [Starukhina, 2001, 2006] :
  - H thermally migrates & diffuse out of crystal to form neutral H exosphere emission or $H_2$ emission
  - H gets trapped in crystal vacancy
  - H creates a local ionization event to immediately react [Poston et al., 2012]
  - Proton reflects from surface back into solar wind [Saito et al., 2008]
- The observation of substantial neutral H emission from the lunar surface [McComas et al., 2009] and $H_2$ [Cook et al., 2013] suggests implantation and outward diffusion is a substantial pathway

# H Implantation & Internal Reactions



Starukhina 2006

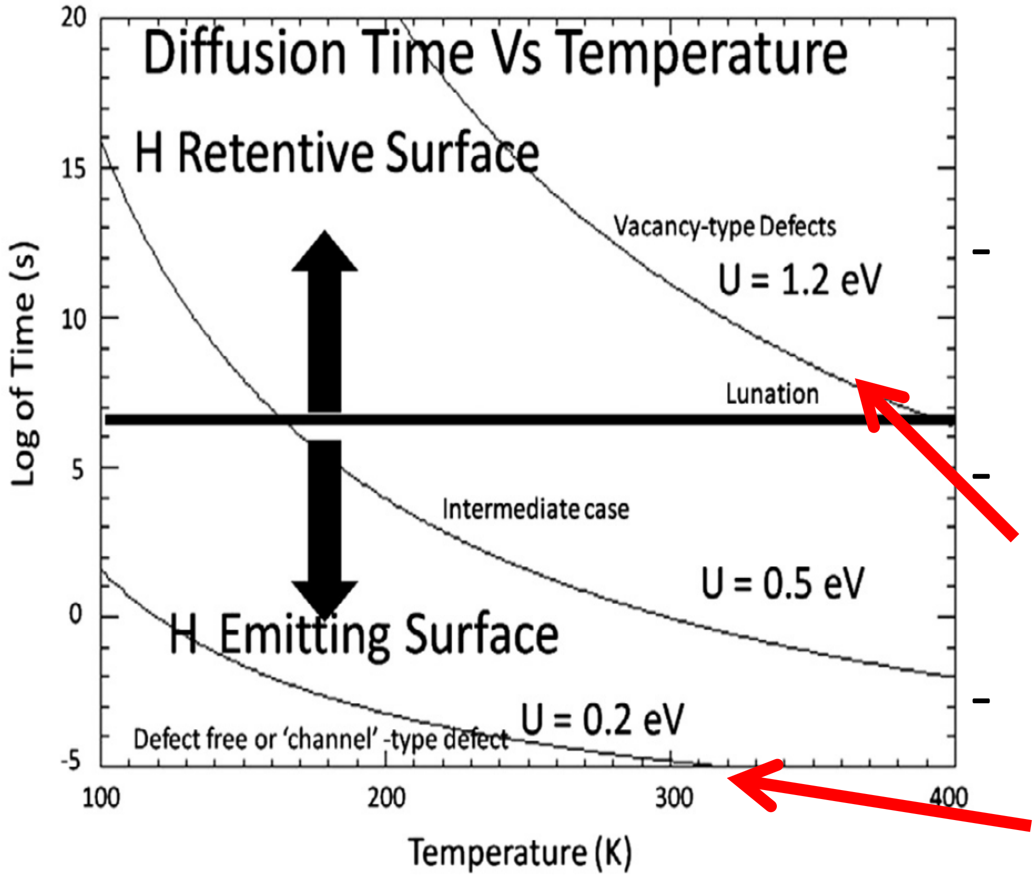
From **Starukhina [2001, 2006, 2012],** an implanted H will migrate from the surface with diffusion time

$$\tau_D = h^2 D_o^{-1} \exp(U/kT)$$

- Depth: h ~$10^{-7}$ m,
- Diffusion $D = D_o \exp(-U/kT)$
- U is diffusion 'activation' energy defining both mobility and trapping of H at a position.
- With defects, U has a range of values, but U > 1 eV in regions leading to trapped or **'loitering'** H's in vacancies

# H Diffusion (or Residency) time

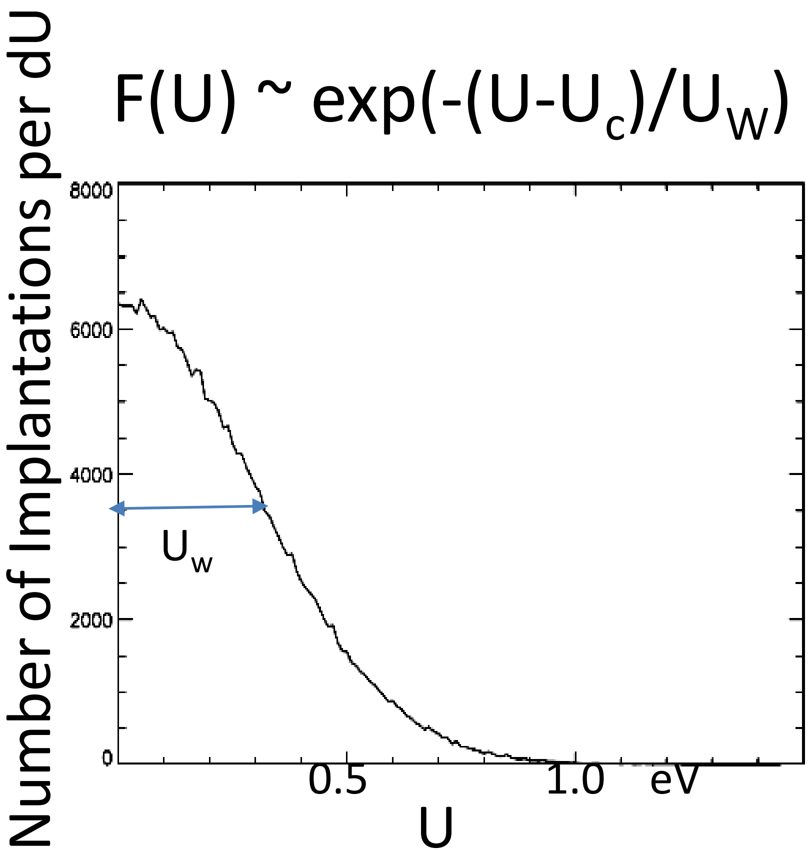
Farrell et al., 2014




Diffusion time as a function of temperature for a family of activation energies, U.

- **Diffusion (outward) time, $\tau_D = h^2 D_o^{-1} \exp(U/kT)$** can also be considered the H residency time
- Residency time is STRONGLY controlled by temperature and activation energy, U
- **High U:** the H can **'loiter'** for 10's of days to possibly form OHs..H retentive surface
- **Low U value:** the H is emitted back out of the surface in seconds ..H emitting surface

# New Statistical Approach: Distribution of Activation Energy




$U_c$ = distribution center,
$U_w$ = distribution width

- For a given sample, the numerous implantations have a **distribution of U values** – not a single U but an **average <U>** and **δU deviation** about the average.
- Expect many of implantations into complete lattice structure (with low U), but some implantations onto lattice with defects represented by higher U
- This statistical view lends itself to a Monte Carlo approach
- We attempt to search for the distribution of U's and temperatures that provides long-lasting, **loitering Hs** ....candidates to form OH.

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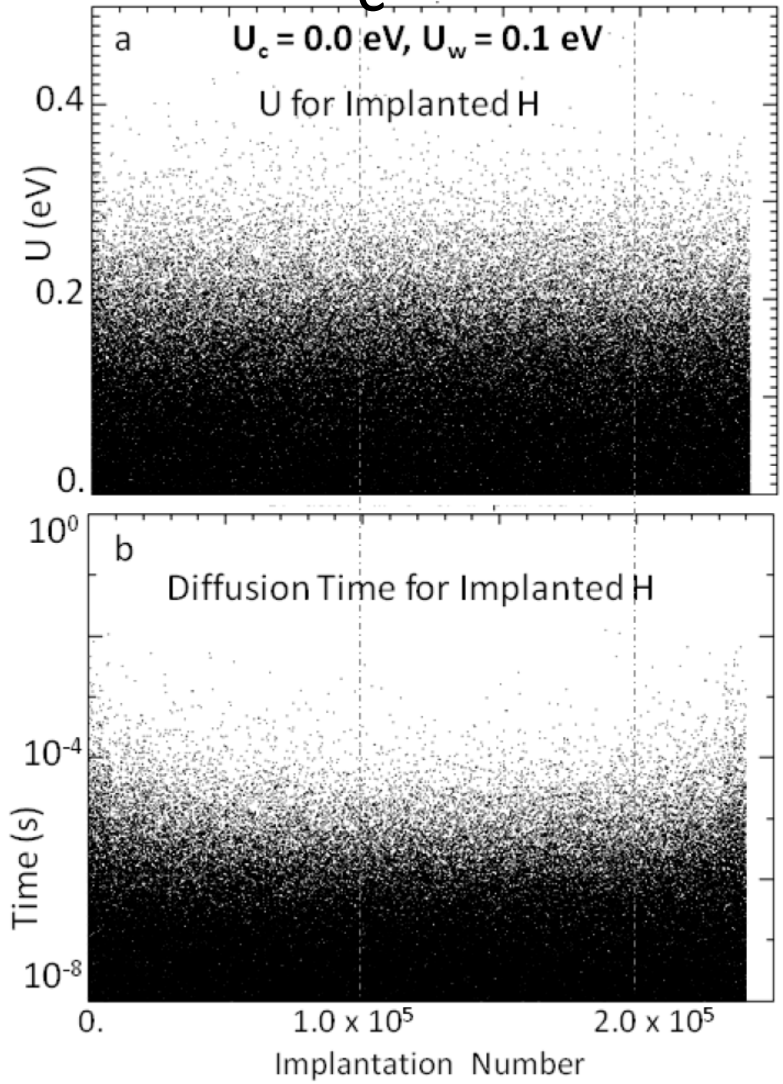
# Methodology

- Divide the lunar equatorial frontside region into local time bins (~1 hour LT or 15$^{o}$ long bins)
- Solar wind ions flux represented by N = 240000 test particles delivered to surface in a flux which varies with local time (i.e., cos of SZA)
- For each implantation, **assign an individual U value quasi-randomly but weighted by a pre-defined Gaussian.**
- We then determine diffusion (residency) time as a function of local surface temperature.
- The number of H's with residency time, $\tau_D > 10^5$ s are considered loitering Hs and **candidates to eventually form OH**. We count these in each local time bin.
  - **H Continuity Eq.:** $dn_H/dt = S - L_{diff} - L_{OH}$
  - **Cold, terminator:** Balance near-terminator solar wind flux, F, onto surface vs estimated amount of OH content from IR observations:

    $$\mathbf{T > n_{OH}h/F > 10^5\ s}$$ **(cannot be much longer than a ¼ lunation)**
- We thus examine the conditions to obtain substantial amounts of these 'loitering', long-lasting Hs that are candidates to form OH.
- Example cases now shown

# Case A: $U_c = 0$ eV , $U_w = 0.1$ eV




U

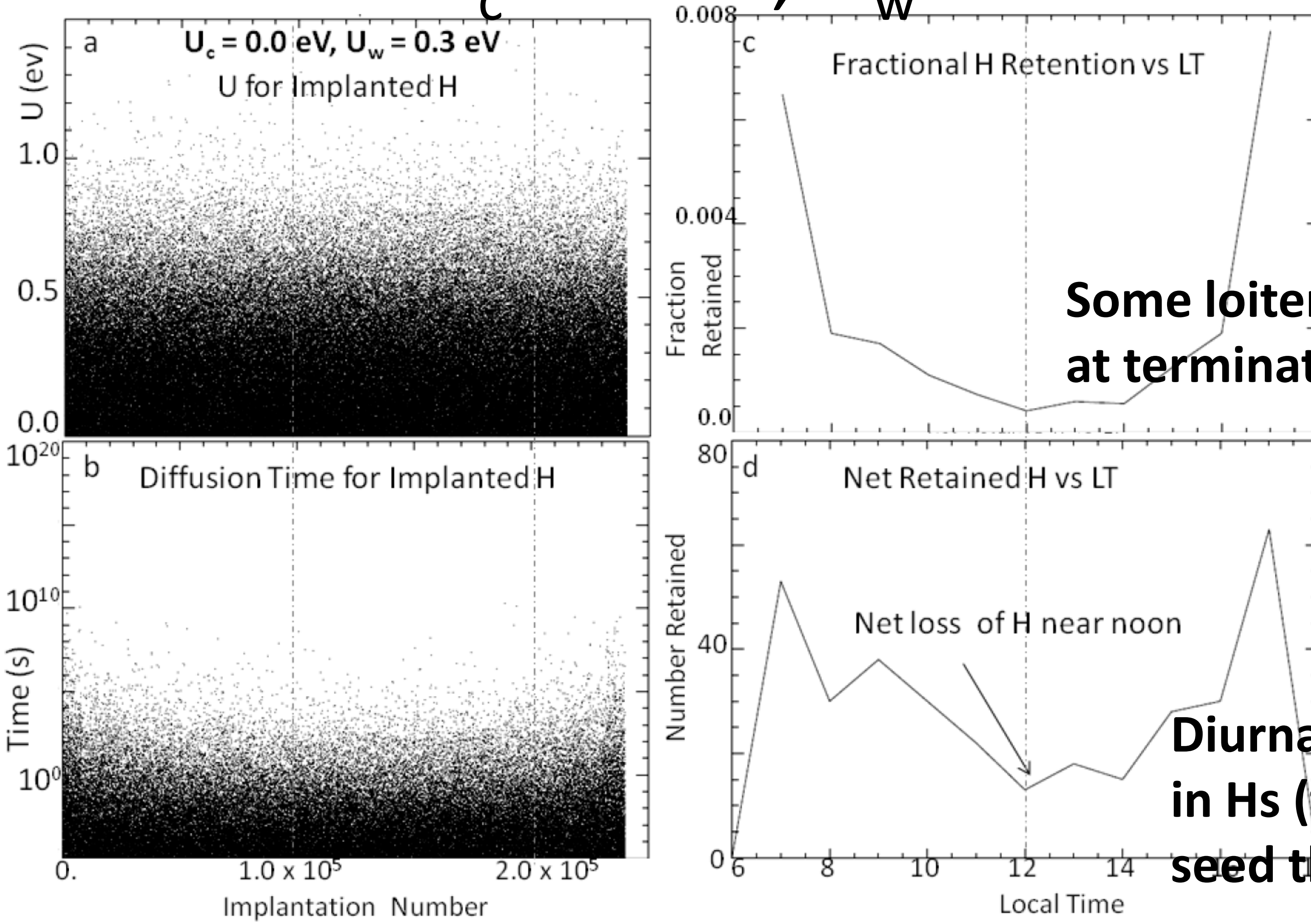
Nearly defect free lattice with low U values

**No loitering H's!**

-Most of implantations have activation energies below 0.4 eV.

-Retention time/loitering time of H's less than 1 second at all locations – all H's lost, no OH.

# Case B: $U_c$ = 0 eV , $U_w$ = 0.3 eV



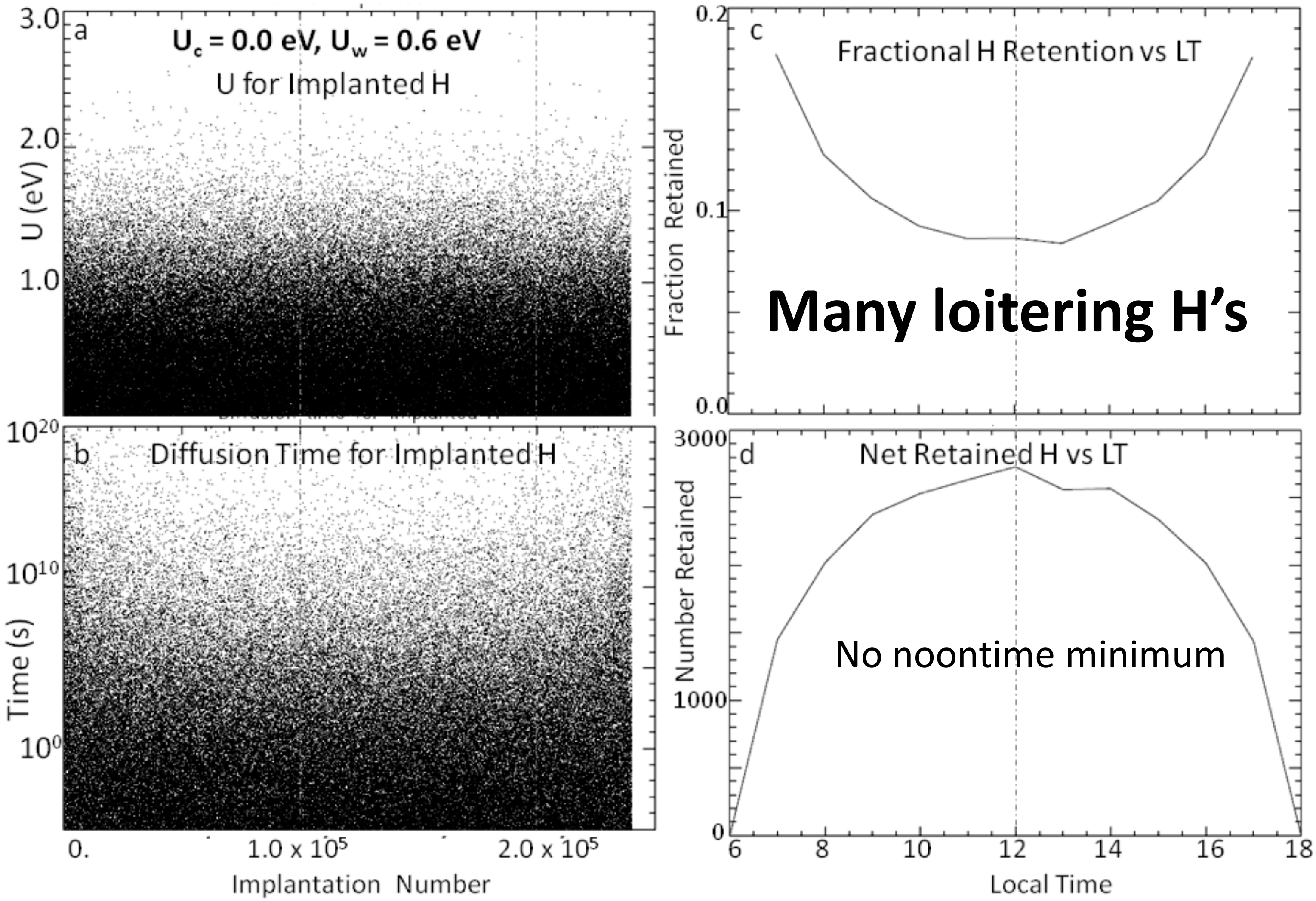

**Some loitering H's at terminators**

**Diurnal effect in Hs (that seed the OH)**

-Only at the terminators is there a substantial population of loitering Hs

-The warmer regolith near noon releases the Hs, possibly creating a neutral H exosphere

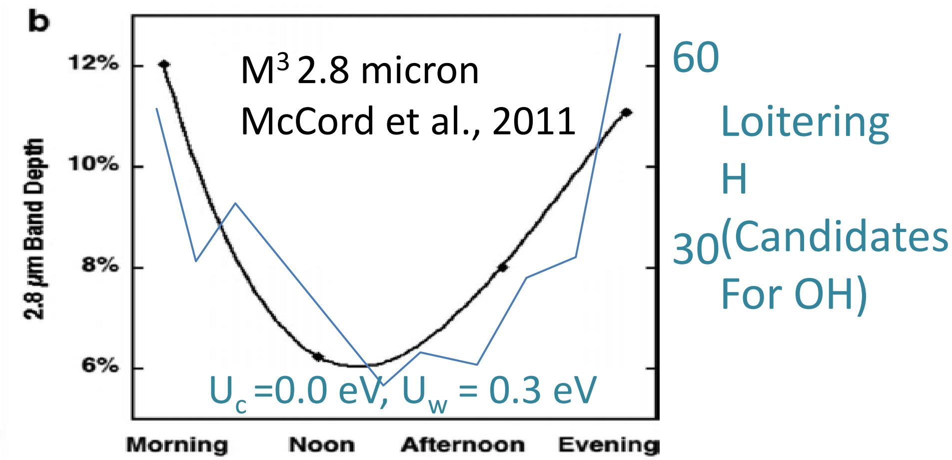
# Case C: $U_c$ = 0 eV , $U_w$ = 0.6 eV




-Substantial population of loitering Hs even at warm noontime

-Still noontime loss via diffusion, but the loss is offset by greater retention at numerous defects sites

# Comparison to the Moon




- Clark et al. 2009: Mild retention of OH (well below saturation) at 10-1000 ppm (over long term)
- Sunshine et al 2009: Reduction in OH at sub-solar point
- Consistent with H implantations having $U_c$ < 0.3 eV, $U_w$ < 0.2 eV

**Table 1**

Values of total fraction retained and the relative retention at noon LT (compared to 8 h LT) for a set of runs under varying $U_c$ and $U_w$ for a thermal profile like that at the lunar equator. Bold values indicate $U_c/U_w$ values where a local noontime minimum is modeled. The shaded values are $U_c/U_w$ values that could be similar to the Moon's mild retention (see text for further discussion).

| | $U_c$ = 0.0 eV | | $U_c$ = 0.3 eV | | $U_c$ = 0.6 eV | | $U_c$ = 0.9 eV | |
|---|---|---|---|---|---|---|---|---|
| $U_w$= 0.1 eV | 0.0 | 0.0 | 0.0 | 0.0 | 0.001 | **-1.0** | 0.22 | **-0.60** |
| $U_w$= 0.2 eV | 0.0 | 0.0 | 0.001 | **-0.64** | 0.034 | **-0.51** | 0.34 | +0.06 |
| $U_w$= 0.3 eV | 0.001 | **-0.56** | 0.013 | **-0.29** | 0.10 | **-0.004** | 0.39 | +0.35 |
| $U_w$= 0.4 eV | 0.016 | **-0.19** | 0.04 | +0.02 | 0.17 | +0.27 | 0.42 | +0.51 |
| $U_w$= 0.6 eV | 0.10 | +0.35 | 0.14 | +0.41 | 0.27 | + 0.53 | 0.45 | +0.67 |
| Uw=0.75 eV | 0.19 | +0.54 | 0.22 | +0.56 | 0.33 | +0.63 | 0.46 | +0.72 |
| $U_w$= 0.9 eV | 0.27 | +0.64 | 0.30 | +0.65 | 0.37 | +0.70 | 0.48 | +0.76 |

# 3 Classes of Implantations

| | U (eV) | Diffusion time (s) | Loss from surface via | Observed in | Observed via |
|---|---|---|---|---|---|
| **Low U** | < 0.3 | < $10^1$ | Quick diffusion | Emitted H or $H_2$ | IBEX, LAMP |
| **Intermediate U** | 0.3 to 0.9 | $10^2$ - $10^{14}$ | Diurnal –scale thermal diffusion | Surface | IR (e.g., $M^3$ ) |
| **High U** | > 0.9 | $10^7$ To over $10^{16.5}$ | Impactors | Surface | IR (e.g., $M^3$ ) |

- Model a continuum in U but ‘classes’ based on loss process

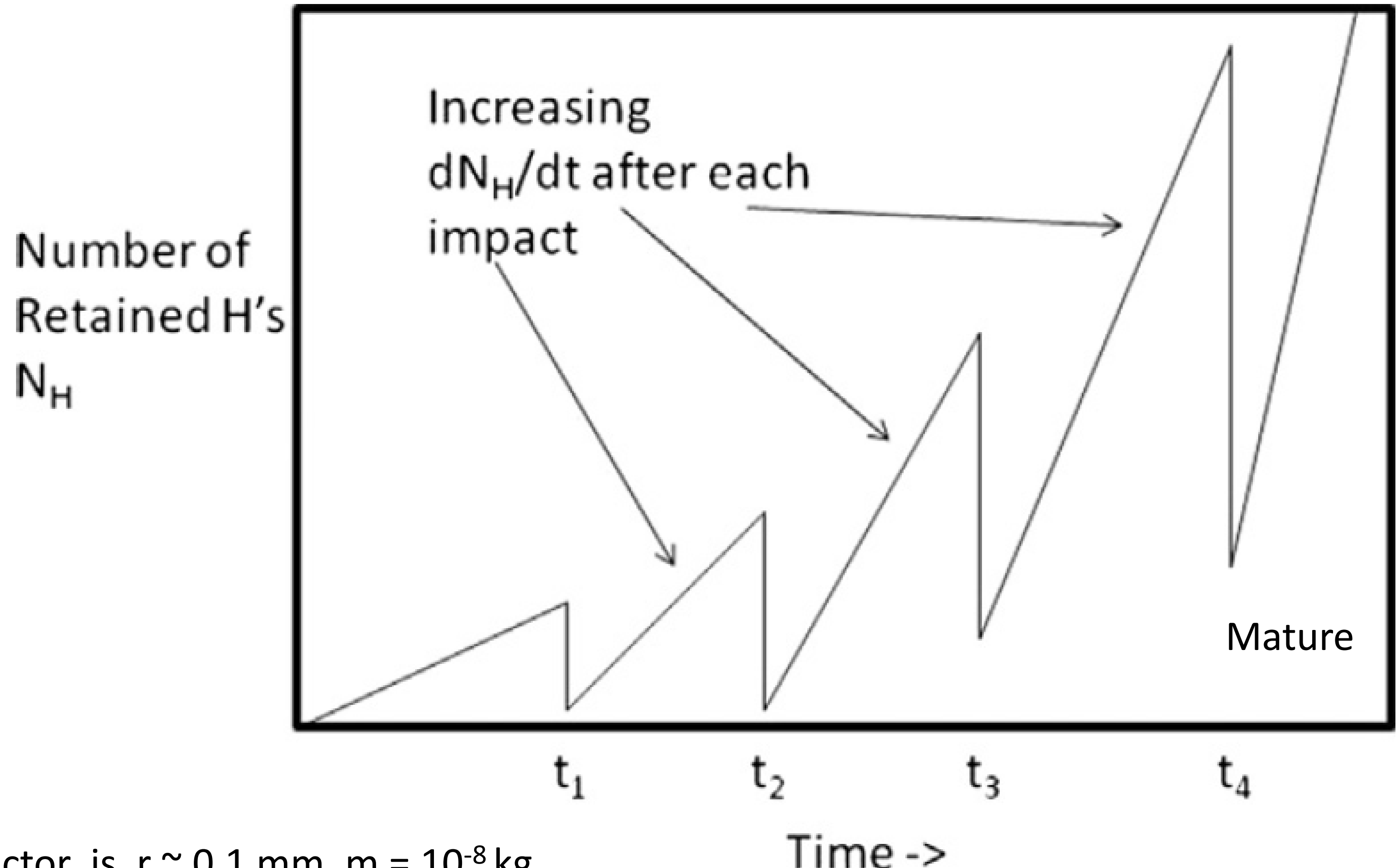
-We propose that **impactors** as a loss process regulate the amount of long-term loitering H

-**Micro-meteoroids** act to ‘reset’ the affected regolith by releasing H’s and by adding defects to make the surface more retentive.

-Keep surface from becoming saturated by ‘impact-reset’ (Over long term, see only 10-1000 ppm –well below saturation)

-Look at U/T: Explains both thermal effect and increase H in mature (highland) soils

# Illustration of Implantation history of a 1 mm x 1mm area




Impactor is r ~ 0.1 mm, m = $10^{-8}$ kg
Impacts a 1 mm x 1mm region every $10^5$ years.

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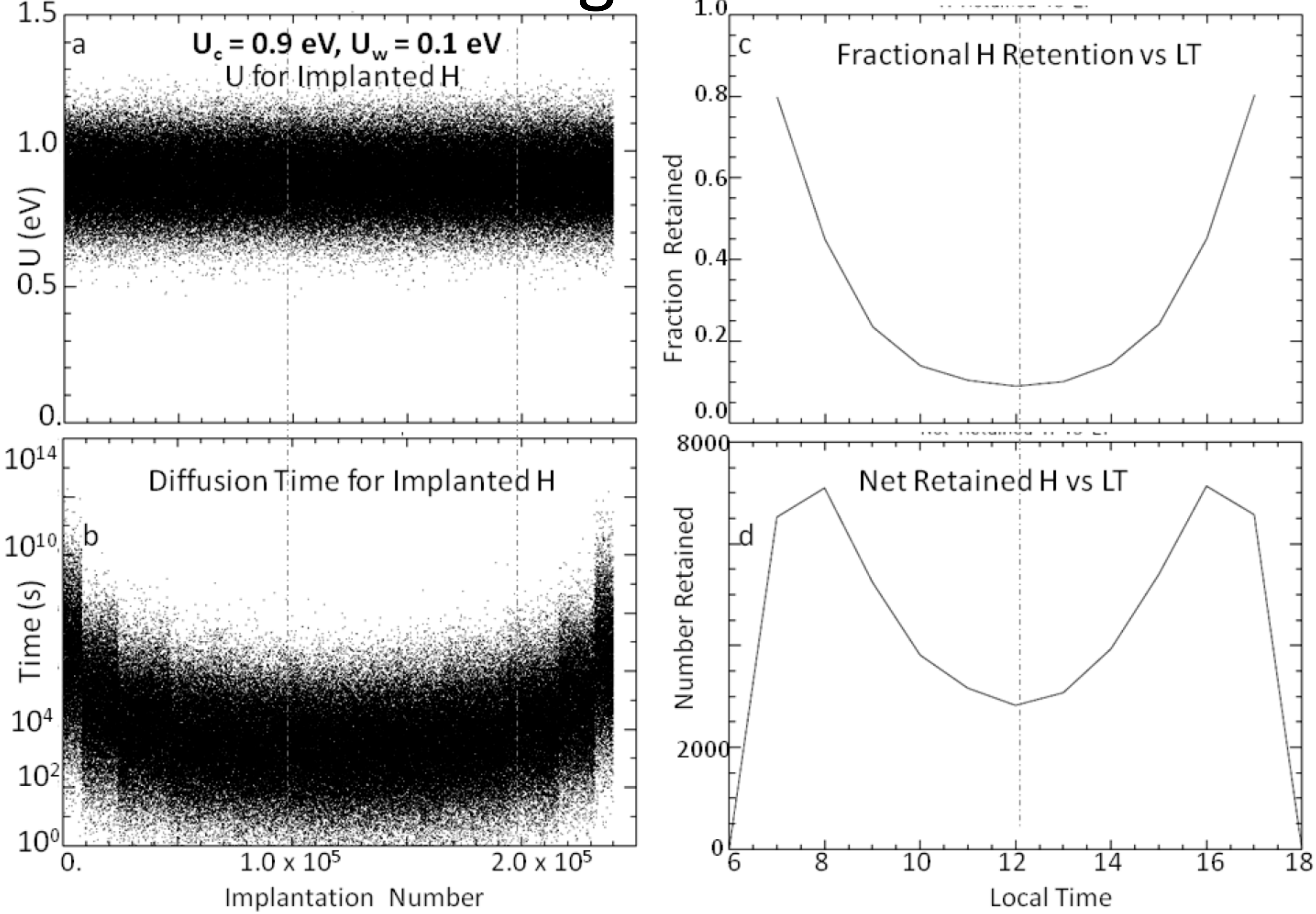
# Conclusions

- The **defect properties of a crystal** has as much (or more) control on solar wind H retention in an exposed regolith as temperature and solar wind influx
- **U/T** is the primary variable in residency, not just T
  - T varies by a factor of 4, U varies by a factor of 100
  - T appears as a controlling variable only at intermediate U values
- The nature of the crystal may be a variable in H retention and OH formation that is **under-appreciated**.
- Focus on U/T: Can explain a diurnal cycle to H and also increased retention in mature soils (lunar highlands)
- We use Gaussian's to illustrate of effect but real crystal defect distribution (U distribution) likely more complicated (e.g., amorphized rims - Noble et al., 2005)
- Starukhina's work pioneering
- Extended discussion in recent Icarus paper!

# backup

# Interesting Test Case



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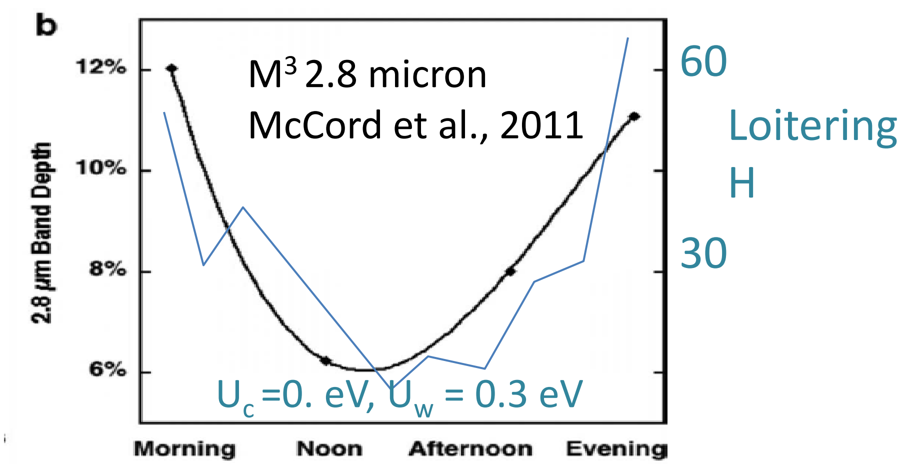


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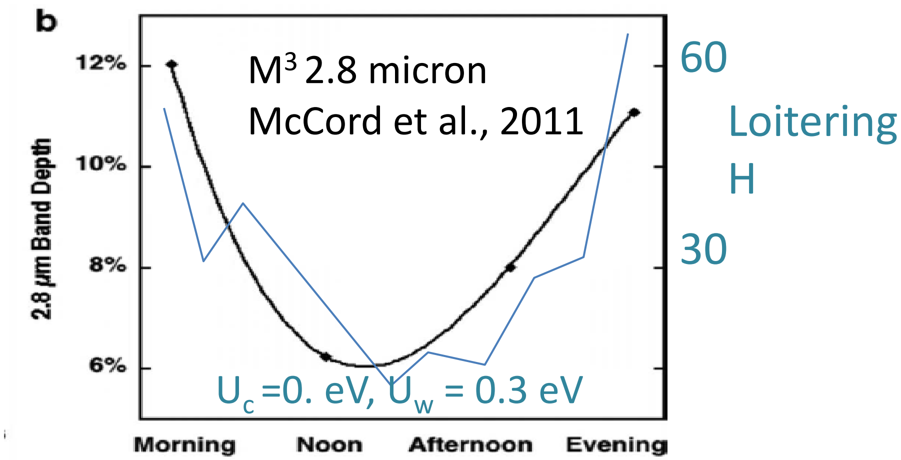
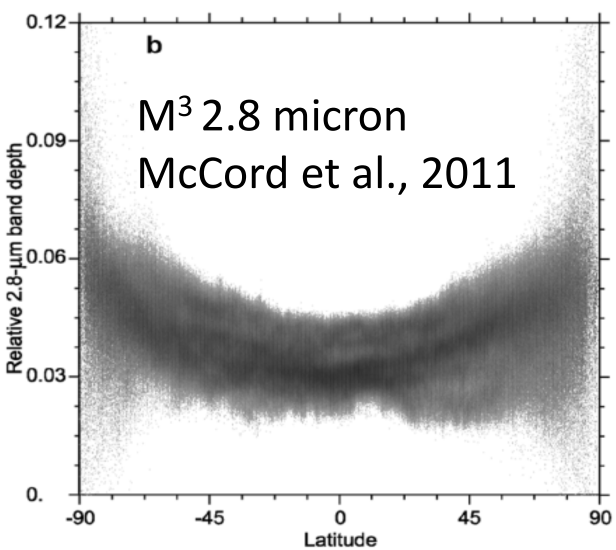
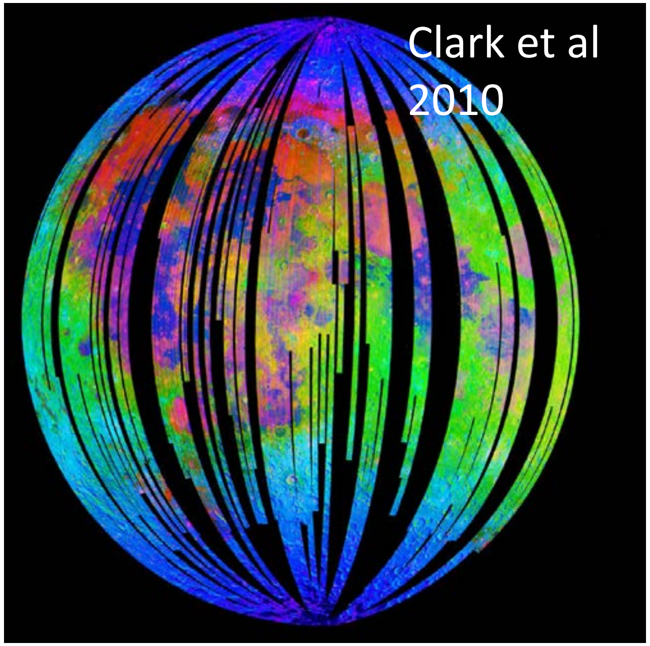



- Mild retention (well below saturation)
- Reduction in H (and hence OH) at sub-solar point
- Consistent with $U_c < 0.3$ eV, $U_w < 0.2$ eV
- Have a fraction of implantations with 0.3 eV < U < 0.9 eV

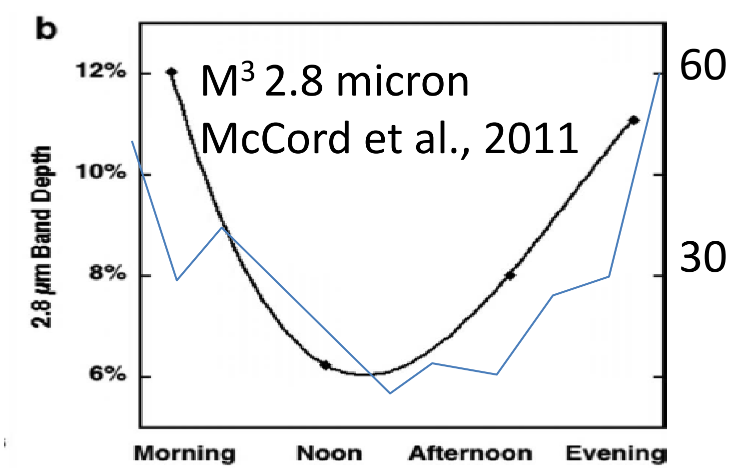


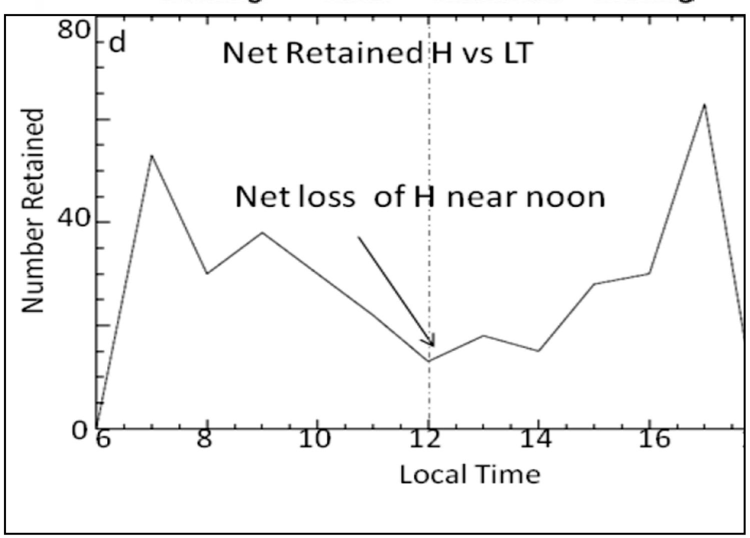



# Comparison to Moon

H's Retained

- Mild retention
- Reduction in H (and hence OH) at sub-solar point
- Consistent with $U_c < 0.3$ eV, $U_w < 0.2$ eV
- Have a fraction of implantations with $0.3 \text{ eV} < U < 0.9 \text{ eV}$




$U_c$ =0. eV, $U_w$ = 0.3 eV